MONKES: a fast neoclassical code for stellarators

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April 2023

Abstract.

Keywords: Neoclassical transport, stellarator optimization, bootstrap current.
Submitted to: *Nucl. Fusion*

1. Introduction

2. Drift-kinetic equation and transport coefficients

In this section, we will describe the drift-kinetic equation that `MONKES` solves and the transport coefficients that can be computed once it is solved. For the spatial domain, we will employ Boozer coordinates $(\psi, \theta, \zeta) \in [0, \psi_{\text{lcfs}}] \times [0, 2\pi) \times [0, 2\pi/N_p)$ where ψ is the flux-surface label, $2\pi\psi$ is the toroidal flux of the magnetic field and θ, ζ are respectively the poloidal and toroidal (in a single period) angles. The integer $N_p \geq 1$ denotes the number of periods of the device. In these coordinates the magnetic field can be written as

$$\begin{aligned} \boldsymbol{B} &= \nabla\psi \times \nabla\theta - \iota(\psi)\nabla\psi \times \nabla\zeta \qquad (1)\\ &= B_\psi(\psi,\theta,\zeta)\nabla\psi + B_\theta(\psi)\nabla\theta + B_\zeta(\psi)\nabla\zeta, \end{aligned}$$

and the Jacobian of the transformation reads

$$\sqrt{g}(\psi,\theta,\zeta) := (\nabla\psi \times \nabla\theta \cdot \nabla\zeta)^{-1} = \frac{B_\zeta + \iota B_\theta}{B^2}, \quad (2)$$

where we have denoted $B := |\boldsymbol{B}|$ and $\iota = \boldsymbol{B}\cdot\nabla\theta/\boldsymbol{B}\cdot\nabla\zeta$ is the rotational transform.

The new code `MONKES` solves numerically the drift-kinetic equation presented in [1] using as velocity coordinates the cosine of the pitch-angle $\xi := \boldsymbol{v}\cdot\boldsymbol{b}/|\boldsymbol{v}|$ and the module of the velocity $v := |\boldsymbol{v}|$ where $\boldsymbol{b} = \boldsymbol{B}/B$. The equation for the specie a of charge e_a and mass m_a in these coordinates reads

$$(v\xi\boldsymbol{b} + \boldsymbol{v}_E)\cdot\nabla F_a + v\nabla\cdot\boldsymbol{b}\frac{(1-\xi^2)}{2}\frac{\partial F_a}{\partial\xi} - \nu^a(v)\mathcal{L}F_a = S_a. \quad (3)$$

Here,

$$\boldsymbol{v}_E = \frac{\boldsymbol{E}_0 \times \boldsymbol{B}}{\langle B^2\rangle} = \Phi_0'(\psi)\frac{\boldsymbol{B}\times\nabla\psi}{\langle B^2\rangle}, \quad (4)$$

is the incompressible $\boldsymbol{E}\times\boldsymbol{B}$ drift approximation,

$$\mathcal{L} = \frac{1}{2}\frac{\partial}{\partial\xi}\left((1-\xi^2)\frac{\partial}{\partial\xi}\right) \quad (5)$$

is the Lorentz pitch-angle scattering operator. In the collision operator, $\nu^a(v) = \sum_b \nu^{ab}(v)$ and

$$\nu^{ab}(v) = \frac{4\pi n_b e_a^2 e_b^2}{m_a^2 v_{\text{ta}}^3}\log\Lambda\frac{\operatorname{erf}(v/v_{\text{tb}}) - G(v/v_{\text{tb}})}{v^3/v_{\text{ta}}^3}, \quad (6)$$

stands for the pitch-angle collision frequency between species a and b, we denote by $G(x) = \left[\operatorname{erf}(x) - (2x/\sqrt{\pi})\exp(-x^2)\right]/(2x^2)$ to the Chandrasekhar function, $\log\Lambda$ is the Coulomb logarithm, $n_b(\psi)$ is the density of specie b, $v_{\text{ta}}^2 = 2T_a(\psi)/m_a$ is the thermal velocity of specie a and T_a its temperature in energy units.

In the right-hand-side of (3)

$$S_a = -\boldsymbol{v}_{\text{ma}}\cdot\nabla\psi f_{\text{Ma}}\left(A_{1a} + \frac{v^2}{v_{\text{ta}}^2}A_{2a}\right) - Bv\xi A_{3a}f_{\text{Ma}}, \quad (7)$$

is the source term,

$$\boldsymbol{v}_{\text{ma}}\cdot\nabla\psi = -\frac{Bv^2}{\Omega_a}\frac{1+\xi^2}{2B^3}\boldsymbol{B}\times\nabla\psi\cdot\nabla B, \quad (8)$$

is the magnetic radial drift, $\Omega_a = e_a B/m_a$ is the gyrofrecuency, the flux functions

$$A_{1a}(\psi) = \frac{n_a'}{n_a} - \frac{3}{2}\frac{T_a'}{T_a} + \frac{e_a\Phi_0'}{T_a}, \quad (9)$$

$$A_{2a}(\psi) = \frac{T_a'}{T_a}, \quad (10)$$

$$A_{3a}(\psi) = -\frac{e_a}{T_a}\frac{\langle\boldsymbol{E}\cdot\boldsymbol{B}\rangle}{\langle B^2\rangle}, \quad (11)$$

are the thermodinamical forces and

$$f_{\text{Ma}}(\psi,v) = n_a(\psi)\pi^{-3/2}v_{\text{ta}}^{-3}(\psi)\exp\left(-\frac{v^2}{v_{\text{ta}}^2(\psi)}\right), \quad (12)$$

is a Maxwellian distribution. Here, the symbol $\langle ...\rangle$ stands for the flux-surface average operation, which in Boozer coordinates (θ,ζ) takes the form

$$\langle F\rangle = \frac{1}{V'(\psi)}\oint\oint\sqrt{g}(\psi,\theta,\zeta)F(\psi,\theta,\zeta)\,\mathrm{d}\theta\,\mathrm{d}\zeta \quad (13)$$

for any well-behaved function $F(\psi,\theta,\zeta)$ and $V'(\psi)$ is fixed from the condition $\langle 1\rangle = 1$. Also, the spatial differential operators involved in (3) in Boozer coordinates take the form

$$\boldsymbol{b}\cdot\nabla = \frac{B}{B_\zeta + \iota B_\theta}\left(\frac{\partial}{\partial\zeta} + \iota\frac{\partial}{\partial\theta}\right), \quad (14)$$

$$\boldsymbol{B}\times\nabla\psi\cdot\nabla = \frac{B^2}{B_\zeta + \iota B_\theta}\left(B_\zeta\frac{\partial}{\partial\theta} - B_\theta\frac{\partial}{\partial\zeta}\right). \quad (15)$$

The radial locality of the drift-kinetic equation (3) comes from neglecting both the component of $\boldsymbol{E}$ tangential to the flux-surface and the magnetic drift in the Vlasov operator, which accounts for the dynamics of particles in phase space in the absence of collisions. Thus, there are no derivatives of F_a along ψ in (3). Such drift-kinetic equation is called monoenergetic as collisionless trajectories preserve both the total energy $E_a = m_a v^2/2 + e_a\Phi_0(\psi)$ and the kinetic energy $K_a := m_a v^2/2$. Indeed, along their collisionless movement, conservation of E_a implies

$$\dot{K}_a = -e_a\Phi_0'(\psi)\nabla\psi\cdot(v\xi\boldsymbol{b} + \boldsymbol{v}_E) = 0. \quad (16)$$

However, unlike rigorous derivations of guiding center trajectories (see e.g. [2, 3]), the magnetic moment $\mu_a := K_a(1-\xi^2)/B$ is conserved only for $E_\psi = 0$, that is, $\dot{\mu}_a = \mu_a B \boldsymbol{v}_E \cdot \nabla(1/B)$ is non zero in terms of the order of the normalized gyrorradius $v_{\mathrm{t}a}/\Omega_a$. Due to the exclusion of the magnetic drift, this model does not account for resonant superbanana orbits, which appear when the $\boldsymbol{E} \times \boldsymbol{B}$ and magnetic drifts compensate each other. Nevertheless, this drift-kinetic equation model retains the poloidal precession due to the radial electric field, and therefore transition particles. This trajectory model is included, for instance, in the standard neoclassical code `DKES` [4] or the more recent Fokker-Planck code `SFINCS` [5]. Moreover, in [6] it is proven that the orbit averaged version of (3) is correct at low collisionality for large aspect ratio stellarators. The equation presented in [6] is solved to calculate radial transport by the fast neoclassical code `KNOSOS` [7].

The solution of (3) is determined up to a function of (ψ, v) as the drift-kinetic equation has a nullspace spanned by any function $g(\psi, v)$. This function is unimportant as it does not contribute to the transport coefficients but nevertheless, in order to have a unique solution to the drift-kinetic equation it must be fixed imposing an appropriate additional constraint. A possible selection is to impose that the distribution function takes a fixed value at a particular phase-space point. Another selection (for fixed (ψ, v)) could be to impose

$$\left\langle \int_{-1}^{1} F_a \,\mathrm{d}\xi \right\rangle = C, \tag{17}$$

for some $C \in \mathbb{R}$.

Now we will give the drift-kinetic equation in the form in which `MONKES` solves it to calculate the transport coefficients. The idea is to write the equation in a form in which depends only on the magnetic configuration and not on the species. Thus, we can write the radial and parallel transport quantities (which are of course species dependant) in terms of what we call monoenergetic geometric coefficients, which for fixed $(\hat{\nu}, \hat{E}_\psi)$ depend only on the magnetic configuration. As equation (3) does not couple the distribution function of different species, we can drop the index a. Besides, as it is linear in F_a, we can decompose its solution using superposition. We split (3) in three equations

$$\xi \boldsymbol{b} \cdot \nabla f_i + \nabla \cdot \boldsymbol{b} \frac{(1-\xi^2)}{2} \frac{\partial f_i}{\partial \xi} - \frac{\hat{E}_\psi}{\langle B^2 \rangle} \boldsymbol{B} \times \nabla\psi \cdot \nabla f_i - \hat{\nu} \mathcal{L} f_i = s_i, \tag{18}$$

for $i = 1, 2, 3$, where $\hat{\nu} := \nu(v)/v$ and $\hat{E}_\psi := -\Phi_0'(\psi)/v$.

The source terms are given by

$$s_1 = -\boldsymbol{v}_{\mathrm{m}a} \cdot \nabla\psi \frac{\Omega_a}{Bv^2}, \quad s_2 = s_1, \quad s_3 = -\xi B. \tag{19}$$

The solution F_a to (3) is related to the functions f_i via

$$F_a = f_{\mathrm{M}a} \left[\frac{Bv}{\Omega_a} \left(A_{1a} f_1 + A_{2a} \frac{v^2}{v_{\mathrm{t}a}^2} f_2 \right) + A_{3a} f_3 \right]. \tag{20}$$

Note that for fixed $(\hat{\nu}, \hat{E}_\psi)$, equation (18) is completely determined by the magnetic configuration. Specifically, the magnetic configuration enters through the flux functions B_θ, B_ζ, ι, the magnetic field strength B and its derivatives along θ and ζ. As $\mathrm{d}\hat{\nu}/\mathrm{d}v$ never annuls, the dependence of f_1 on the velocity v can be parametrized by its dependence on $\hat{\nu}$. Thus, for a fixed value of $\hat{\nu}$, fixing a value of $\hat{E}_\psi$ is equivalent to selecting a value of radial electric field.

Taking the moments $\{\boldsymbol{v}_{\mathrm{m}a} \cdot \nabla\psi, (v^2/v_{\mathrm{t}a}^2)\boldsymbol{v}_{\mathrm{m}a} \cdot \nabla\psi, v\xi B\}$ of F_a and then the flux-surface average yield respectively the radial particle and heat fluxes and the parallel flow

$$\langle \boldsymbol{\Gamma}_a \cdot \nabla\psi \rangle = \left\langle \int \boldsymbol{v}_{\mathrm{m}a} \cdot \nabla\psi F_a \,\mathrm{d}^3\boldsymbol{v} \right\rangle \tag{21}$$

$$\left\langle \frac{\boldsymbol{Q}_a \cdot \nabla\psi}{T_a} \right\rangle = \left\langle \int \frac{v^2}{v_{\mathrm{t}a}^2} \boldsymbol{v}_{\mathrm{m}a} \cdot \nabla\psi F_a \,\mathrm{d}^3\boldsymbol{v} \right\rangle \tag{22}$$

$$\langle n_a \boldsymbol{V}_a \cdot \boldsymbol{B} \rangle = \left\langle B \int v\xi F_a \,\mathrm{d}^3\boldsymbol{v} \right\rangle \tag{23}$$

Using (20) we can write them in matricial form

$$\begin{bmatrix} \langle \boldsymbol{\Gamma}_a \cdot \nabla\psi \rangle \\ \left\langle \dfrac{\boldsymbol{Q}_a \cdot \nabla\psi}{T_a} \right\rangle \\ \langle n_a \boldsymbol{V}_a \cdot \boldsymbol{B} \rangle \end{bmatrix} = \begin{bmatrix} L_{11a} & L_{12a} & L_{13a} \\ L_{21a} & L_{22a} & L_{23a} \\ L_{31a} & L_{32a} & L_{33a} \end{bmatrix} \begin{bmatrix} A_{1a} \\ A_{2a} \\ A_{3a} \end{bmatrix}. \tag{24}$$

We have defined the thermal transport coefficients as

$$L_{ija} := \int_0^\infty 2\pi v^2 f_{\mathrm{M}a} w_i w_j D_{ija} \,\mathrm{d}v\,, \tag{25}$$

where $w_1 = w_3 = 1$, $w_2 = v^2/v_{\mathrm{t}a}^2$ and we have used that $\int g \,\mathrm{d}^3\boldsymbol{v} = 2\pi \int_0^\infty \int_{-1}^1 g v^2 \,\mathrm{d}\xi \,\mathrm{d}v$ for any integrable gyroaveraged function g. The coefficients D_{ija} are the monoenergetic transport coefficients

$$D_{11a} = D_{12a} = D_{21a} = D_{22a} = \frac{B^2 v^3}{\Omega_a^2} \Gamma_{11}, \tag{26}$$

$$D_{13a} = D_{23a} = \frac{Bv^2}{\Omega_a} \Gamma_{13}, \tag{27}$$

$$D_{31a} = D_{32a} = \frac{Bv^2}{\Omega_a} \Gamma_{31}, \tag{28}$$

$$D_{33a} = v\Gamma_{33}, \tag{29}$$

and Γ_{ij} are the monoenergetic geometric coefficients given by

$$\Gamma_{ij}(\psi, v) = \left\langle \int_{-1}^{1} s_i f_j \,\mathrm{d}\xi \right\rangle, \quad i, j \in \{1, 2, 3\}. \qquad (30)$$

Note that the monoenergetic geometric coefficients Γ_{ij} do not depend on the species for fixed $\hat{\nu}$ (however the correspondent value of v associated to each $\hat{\nu}$ varies between species) and depend only on the magnetic geometry. Of the monoenergetic geometric coefficients Γ_{ij} only 3 of them are independent as Onsager symmetry implies $\Gamma_{13} = -\Gamma_{31}$. Hence, to obtain the transport coefficients for all species, requires to solve (18) for 2 different source terms s_1 and s_3. The algorithm for inverting approximately the left-hand-side of (18) to any degree of accuracy is described in the next section.

3. Algorithm

In this section we describe the algorithm implemented to numerically solve the drift-kinetic equation. As we are not going to do it for a particular source term, but instead a general one, we drop the subscript i that labels every different source term when possible. Also, as ψ and v act as mere parameters we will omit their dependence in this section and functions of these two variables will be referred as constants. The algorithm is based on the approximate representation of the distribution function f in a truncated Legendre series. We will search for approximate solutions to (18) of the form

$$f(\theta, \zeta, \xi) = \sum_{k=0}^{N_\xi} f^{(k)}(\theta, \zeta) P_k(\xi). \qquad (31)$$

In Appendix A we derive explicitly the projection of each term of (18) onto the Legendre basis when the representation (31) is used. When doing so, we get that the Legendre modes of the drift-kinetic equation have the well known [1] tridiagonal representation

$$L_k f^{(k-1)} + D_k f^{(k)} + U_k f^{(k+1)} = s^{(k)}, \qquad (32)$$

for $k = 0, 1, \ldots, N_\xi$, where we have defined for convenience $f^{(-1)} := 0$ and from expansion (31) is clear that $f^{(N_\xi+1)} = 0$. The spatial differential operators read

$$L_k = \frac{k}{2k-1}\left(\boldsymbol{b}\cdot\nabla + \frac{k-1}{2}\boldsymbol{b}\cdot\nabla \ln B\right), \qquad (33)$$

$$D_k = -\frac{\hat{E}_\psi}{\langle B^2\rangle}\boldsymbol{B}\times\nabla\psi\cdot\nabla + \frac{k(k+1)}{2}\hat{\nu}, \qquad (34)$$

$$U_k = \frac{k+1}{2k+3}\left(\boldsymbol{b}\cdot\nabla - \frac{k+2}{2}\boldsymbol{b}\cdot\nabla \ln B\right). \qquad (35)$$

Thanks to its tridiagonal structure, the system (32) can be formally inverted using the standard Gaussian elimination algorithm for block tridiagonal matrices. Before introducing the algorithm we will explain how to fix the free constant of (32) so that it can be inverted. Note that the aforementioned nullspace of the drift-kinetic equation traduces in the fact that $f^{(0)}$ is not completely determined from (32). To prove this, we inspect the modes $k = 0$ and $k = 1$ that involve $f^{(0)}$. The equation $D_0 f^{(0)} + U_0 f^{(1)}$ is invariant if we add to $f^{(0)}$ any function of $B_\theta\zeta + B_\zeta\theta$ when $\hat{E}_\psi \neq 0$ and does not include $f^{(0)}$ for $\hat{E}_\psi = 0$. Besides, the equation $L_1 f^{(0)} + D_1 f^{(1)} + U_1 f^{(2)}$ remains invariant if we add to $f^{(0)}$ any constant. Thus, we get that (32) is unaltered when we add to $f^{(0)}$ a constant. A condition equivalent to (17) is to fix the value of the $0-$th Legendre mode of the distribution function at a point of the flux-surface. For example,

$$f^{(0)}(0, 0) = 0. \qquad (36)$$

With this condition, (32) has a unique solution and can be inverted (further details on the invertibility are given in Appendix B) to obtain an approximation of the first $N_\xi + 1$ Legendre modes of the exact solution to (18). The algorithm for formally solving (32) consists of two steps.

(i) **Forward elimination**

Starting from $\Delta_{N_\xi} = D_{N_\xi}$ and $\sigma^{(N_\xi)} = s^{(N_\xi)}$ we can obtain recursively the operators

$$\Delta_k = D_k - U_k \Delta_{k+1}^{-1} L_{k+1}, \qquad (37)$$

for $k = N_\xi - 1, N_\xi - 2, \ldots, 0$ and transform (32) to the equivalent system

$$L_k f^{(k-1)} + \Delta_k f^{(k)} = \sigma^{(k)}, \qquad (38)$$

for $k = 0, 1, \ldots, N_\xi$ where

$$\sigma^{(k)} = s^{(k)} - U_k \Delta_{k+1}^{-1} \sigma^{(k+1)}. \qquad (39)$$

Note that this process corresponds to perform formal Gaussian elimination over

$$\left[\begin{array}{ccc|c} L_k & D_k & U_k & s^{(k)} \\ 0 & L_{k+1} & \Delta_{k+1} & \sigma^{(k+1)} \end{array}\right], \qquad (40)$$

to eliminate U_k in the first row.

(i) **Backward substitution**

Once we have the system of equations in the form (38) it is immediate to solve

$$f^{(k)} = \Delta_k^{-1}\left(\sigma^{(k)} - L_k f^{(k-1)}\right), \qquad (41)$$

for $k = 0, 1, ..., N_\xi$. Here, we denote by $\Delta_0^{-1}\sigma^{(0)}$ to the solution that satisfies (36). Note that for $k = 0$, we must impose condition (36) so that $\Delta_0 f^{(0)} = \sigma^{(0)}$ has a unique solution. As $L_1 = \boldsymbol{b}\cdot\nabla$, it is apparent from (41) that the integration constant does not affect the value of $f^{(1)}$.

We will apply this algorithm to solve approximately (18) for f_1, f_2 and f_3 to compute the transport coefficients. In terms of the Legendre modes of f_1, f_2 and f_3, the monoenergetic geometric coefficients read

$$\Gamma_{11} = 2\left\langle s_1^{(0)} f_1^{(0)}\right\rangle + \frac{2}{5}\left\langle s_1^{(2)} f_1^{(2)}\right\rangle, \tag{42}$$

$$\Gamma_{31} = \frac{2}{3}\left\langle B f_1^{(1)}\right\rangle, \tag{43}$$

$$\Gamma_{13} = 2\left\langle s_1^{(0)} f_3^{(0)}\right\rangle + \frac{2}{5}\left\langle s_1^{(2)} f_3^{(2)}\right\rangle, \tag{44}$$

$$\Gamma_{33} = -\frac{2}{3}\left\langle B f_3^{(1)}\right\rangle, \tag{45}$$

where $3s_1^{(0)}/2 = 3s_1^{(2)} = \boldsymbol{B}\times\nabla\psi\cdot\nabla B/B^3$. Note that, in order to compute the monoenergetic geometric coefficients, we only need to calculate the Legendre modes $k = 0,1,2$ of the solution and we can stop the backward substitution (41) at $k = 2$. The algorithm described above allows, in principle, to compute the exact solution to the truncated drift-kinetic equation (32) which is an approximate solution to (18). However, it is not possible, to our knowledge, to give an exact expression for Δ_k^{-1} except for $k = N_\xi \geq 1$. Instead, we are forced to compute an approximate solution to (32). Discretizing the θ, ζ coordinates in N_θ and N_ζ equispaced points respectively

$$\theta_i = 2\pi i/N_\theta, \qquad i = 0,1,\ldots,N_\theta - 1, \tag{46}$$

$$\zeta_j = 2\pi j/(N_\zeta N_p), \qquad j = 0,1,\ldots,N_\zeta - 1. \tag{47}$$

we can approximate (32) using the Fourier collocation method described in Appendix C and replace (33), (34) and (35) with square matrices of size N_{fs} to obtain the system of equations (C.16). In order to obtain an approximate solution of (32) we shall assume that each $f^{(k)}$ has a finite Fourier spectrum and can be expressed as

$$f^{(k)}(\theta,\zeta) = \boldsymbol{I}(\theta,\zeta)\cdot\boldsymbol{f}^{(k)}, \tag{48}$$

where the vector map $\boldsymbol{I}(\theta,\zeta)$ is defined at Appendix C and $\boldsymbol{f}^{(k)} \in \mathbb{R}^{N_{\text{fs}}}$ contains $f^{(k)}$ evaluated at the grid points (46), (47). When $f^{(k)}$ are given by (48), we can obtain a closed system of equations to determine $\boldsymbol{f}^{(k)}$ by evaluating (32) at the grid points (θ_i,ζ_j) and imposing (36). Hence, our approximations $\{f^{(k)}\}_{k=0}^{N_\xi}$ are the only Fourier interpolants that satisfy (32) at the nodal points and (36). To solve approximately (32), we simply replace in the algorithm the operators L_k, D_k, U_k by the $N_{\text{fs}}\times N_{\text{fs}}$ matrices $\boldsymbol{L}_k$, $\boldsymbol{D}_k$, $\boldsymbol{U}_k$, defined in Appendix C. Applying (37) yields the matrix $\boldsymbol{\Delta}_k$ for which it requires to invert $\boldsymbol{\Delta}_{k+1}$ and multiply matrices. This inversion takes $O(N_{\text{fs}}^3)$ operations using LU factorization and the matrix multiplications involved aswell. For $k \geq 2$, we can reduce the number of matrix multiplications in determining $\boldsymbol{\Delta}_k$ to 1 if instead of computing $\boldsymbol{\Delta}_{k+1}^{-1}$ we solve for $\boldsymbol{X}_{k+1}$ the matrix system of equations

$$\boldsymbol{\Delta}_{k+1}\boldsymbol{X}_{k+1} = \boldsymbol{L}_{k+1}, \tag{49}$$

and then obtain

$$\boldsymbol{\Delta}_k = \boldsymbol{D}_k - \boldsymbol{U}_k\boldsymbol{X}_{k+1}, \tag{50}$$

for $k = N_\xi - 1, N_\xi - 2, \ldots, 2$. For $k \leq 1$ as we need to solve (38) and do the backward substitution (41), it is convenient to compute and store $\boldsymbol{\Delta}_k^{-1}$. As the resolution of a matricial system of equations and matrix multiplication must be done $N_\xi + 1$ times, the inversion of (C.16) by this method requires $O(N_\xi N_{\text{fs}}^3)$ operations. Once we have solved (C.16) for $\boldsymbol{f}^{(0)}$, $\boldsymbol{f}^{(1)}$ and $\boldsymbol{f}^{(2)}$, the integrals of the flux surface average operation involved in the geometric coefficients Γ_{ij}, are computed using the trapezoidal rule, which for periodic analytic functions has geometric convergence [8]. In the next sections we will see that despite the cubic scaling in N_{fs} of the arithmetical complexity of the algorithm, it is possible to obtain fast and accurate calculations of the monoenergetic geometric coefficients (in particular Γ_{31}) in a single processor. The algorithm is implemented in the new code `MONKES`, written in Fortran language. The matrix inversion and multiplication are computed using the linear algebra library `LAPACK` [9].

4. Numerical results and benchmark

5. Conclusions

Appendices

A. Legendre modes of the drift-kinetic equation

Legendre polynomials are the eigenfunctions of the Sturm-Liouville problem in the interval $\xi \in [-1,1]$ defined by the differential equation

$$2\mathcal{L}P_k(\xi) = -k(k+1)P_k(\xi), \tag{A.1}$$

where $k \geq 0$ is an integer, and regularity boundary conditions at $\xi = \pm 1$

$$(1-\xi^2)\frac{\mathrm{d}P_k}{\mathrm{d}\xi}\bigg|_{\xi=\pm 1} = 0. \tag{A.2}$$

As $\mathcal{L}$ has a discrete spectrum and is self-adjoint with respect to the inner product

$$\langle f,g\rangle_{\mathcal{L}} := \int_{-1}^{1} f g \,\mathrm{d}\xi\,, \tag{A.3}$$

in the space of functions that satisfy the regularity condition, $\{P_k\}_{k=0}^{\infty}$ is an orthogonal basis satisfying $\langle P_j, P_k\rangle_{\mathcal{L}} = 2\delta_{jk}/(2k+1)$. Hence, these polynomials satisfy the three-term recurrence formula

$$(2k+1)\xi P_k(\xi) = (k+1)P_{k+1}(\xi) + kP_{k-1}(\xi), \tag{A.4}$$

which starting from $P_0 = 1$ and $P_1 = \xi$ defines them all. Additionally, they satisfy the differential identity

$$(1-\xi^2)\frac{\mathrm{d}P_k}{\mathrm{d}\xi} = kP_{k-1}(\xi) - k\xi P_k(\xi). \tag{A.5}$$

Identities (A.4) and (A.5) are useful to represent tridiagonally the Vlasov operator used in (18) when we use the expansion (31). The $k-$th Legendre mode of the term $\xi\boldsymbol{b}\cdot\nabla f$ is expressed in terms of the modes $f^{(k-1)}$ and $f^{(k+1)}$ using (A.4)

$$\langle \xi\boldsymbol{b}\cdot\nabla f, P_k\rangle_{\mathcal{L}} = \frac{2}{2k+1}\left[\frac{k}{2k-1}\,\boldsymbol{b}\cdot\nabla f^{(k-1)} + \frac{k+1}{2k+3}\,\boldsymbol{b}\cdot\nabla f^{(k+1)}\right]. \tag{A.6}$$

Combining both (A.4) and (A.5) allow to express the $k-$th Legendre mode of the mirror term $\nabla\cdot\boldsymbol{b}((1-\xi^2)/2)\,\partial f/\partial\xi$ in terms of the modes $f^{(k-1)}$ and $f^{(k+1)}$ as

$$\left\langle \frac{1}{2}(1-\xi^2)\nabla\cdot\boldsymbol{b}\frac{\partial f}{\partial\xi}, P_k\right\rangle_{\mathcal{L}} = \frac{\boldsymbol{b}\cdot\nabla\ln B}{2k+1}\left[\frac{k(k-1)}{2k-1}f^{(k-1)} - \frac{(k+1)(k+2)}{2k+3}f^{(k+1)}\right], \tag{A.7}$$

where we have also used $\nabla\cdot\boldsymbol{b} = -\boldsymbol{b}\cdot\nabla\ln B$. The term proportional to $\hat{E}_\psi$ is diagonal in a Legendre representation

$$\left\langle \frac{\hat{E}_\psi}{\langle B^2\rangle}\boldsymbol{B}\times\nabla\psi\cdot\nabla f, P_k\right\rangle_{\mathcal{L}} = \frac{2}{2k+1}\frac{\hat{E}_\psi}{\langle B^2\rangle}\boldsymbol{B}\times\nabla\psi\cdot\nabla f^{(k)}. \tag{A.8}$$

Finally, for the collision operator used in (18), as Legendre polynomials are eigenfunctions of the pitch-angle scattering operator, using (A.1) we obtain the diagonal representation

$$\langle \hat{\nu}\mathcal{L}f, P_k\rangle_{\mathcal{L}} = -\hat{\nu}\frac{k(k+1)}{2k+1}f^{(k)}. \tag{A.9}$$

B. Invertibility of the spatial differential operators

In this Appendix we will study the invertibility of the left-hand-side of (32). For this, we consider L_k, D_k and U_k as operators from the space of smooth functions on the flux-surface $\mathcal{F}$ equipped with the inner product $\langle f,g\rangle_{\mathcal{F}} = \oint\oint fg\,\mathrm{d}\theta\,\mathrm{d}\zeta$ and its induced norm. In this setting L_k, D_k and U_k are bounded operators from $\mathcal{F}$ to $\mathcal{F}$ as all the coefficients are smooth. The operators L_k and U_k given by (33) and (35) do not have a uniquely defined inverse as they have a non zero nullspace. This is a consequence of the fact that the parallel streaming operator

$$\mathcal{V}_\parallel = \xi\boldsymbol{b}\cdot\nabla + \nabla\cdot\boldsymbol{b}\frac{(1-\xi^2)}{2}\frac{\partial}{\partial\xi} \tag{B.1}$$

has a nullspace consisting of functions $g((1-\xi^2)/B)$. Note that we can study the invertibility of L_k and U_k by studying the existence solutions of

$$\frac{\mathrm{d}g}{\mathrm{d}l} + a(l)g = 0, \tag{B.2}$$

which are not identically zero. Here l is the length along magnetic field lines and $a(l)$ is a smooth function over the flux surface. It is easy to check that

$$g(l) = C_h\exp\left(-\int_0^l a(l')\,\mathrm{d}l'\right), \tag{B.3}$$

where $C_h\in\mathbb{R}$. If $C_h\neq 0$, continuity of g on the torus implies that

$$\int_0^{L_c} a(l')\,\mathrm{d}l' = 0, \quad \text{if } \iota\in\mathbb{Q} \tag{B.4}$$

$$\lim_{l\to\infty}\int_0^{l} a(l')\,\mathrm{d}l' = 0, \quad \text{if } \iota\in\mathbb{R}\backslash\mathbb{Q}, \tag{B.5}$$

where L_c is the magnetic field length required for the field line to close itself in a rational surface. On the contrary, if such limit is not 0, C_h must be zero for g to be continuous. Writing the operators L_k and U_k, in the form (B.2) gives $a(l)\propto\partial\ln B/\partial l$, and as $\ln B$ is continuous, either (B.4) or (B.5) is always satisfied. Therefore, the nullspaces of L_k and U_k are not zero, which proves that L_k and U_k are not one-to-one.

Now we will prove that if $\hat{\nu}\neq 0$, all the D_k for $k\geq 1$ are invertible. For $\hat{E}_\psi = 0$, D_k is just a multiplication operator and is obviously invertible if $k\neq 0$. When $\hat{E}_\psi\neq 0$ the proof can be done using a similar argument to the one used for L_k and U_k, as we can transform D_k to an equation superficially very similar to (B.2). First, we change from Boozer angles (ψ,θ,ζ) to a different set of magnetic coordinates $(\tilde{\psi},\alpha,\varphi)$ using the linear transformation

$$\begin{bmatrix} \psi \\ \theta \\ \zeta \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & (1+\iota\delta)^{-1} & \iota \\ 0 & -\delta(1+\iota\delta)^{-1} & 1 \end{bmatrix} \begin{bmatrix} \tilde{\psi} \\ \alpha \\ \varphi \end{bmatrix} \tag{B.6}$$

where $\delta = B_\theta/B_\zeta$. In these coordinates $\boldsymbol{B} = \nabla\tilde{\psi} \times \nabla\alpha = B_{\tilde{\psi}}\nabla\tilde{\psi} + B_\varphi\nabla\varphi$ and

$$\boldsymbol{B} \times \nabla\tilde{\psi} \cdot \nabla f = B^2 \frac{\partial f}{\partial \alpha}. \tag{B.7}$$

Thus, in coordinates (α, φ), the operator D_k takes the form

$$D_k = -\hat{E}_\psi \frac{B^2}{\langle B^2 \rangle} \frac{\partial}{\partial \alpha} + \hat{\nu} \frac{k(k+1)}{2}. \tag{B.8}$$

Hence, we want to prove that

$$-\hat{E}_\psi \frac{B^2}{\langle B^2 \rangle} \frac{\partial g}{\partial \alpha} + \hat{\nu} \frac{k(k+1)}{2} g = s(\alpha, \varphi) \tag{B.9}$$

has a unique solution for any source s. The homogeneous and particular solution to this problem are respectively

$$g_{\mathrm{h}} = G(\varphi) \exp(A_k(\alpha, \varphi)), \tag{B.10}$$

$$g_{\mathrm{p}} = -\frac{\langle B^2 \rangle}{\hat{E}_\psi} \exp(A_k(\alpha, \varphi)) \times \int_0^\alpha s(\alpha', \varphi) \exp(-A_k(\alpha', \varphi)) \frac{\mathrm{d}\alpha'}{B^2(\alpha', \varphi)} \tag{B.11}$$

where $G(\varphi)$ is an integration constant and

$$A_k(\alpha, \varphi) = \hat{\nu} \frac{k(k+1)}{2} \frac{\langle B^2 \rangle}{\hat{E}_\psi} \int_0^\alpha \frac{\mathrm{d}\alpha''}{B^2(\alpha'', \varphi)}. \tag{B.12}$$

Note from (B.6), that the curves of constant φ are straight lines in the (θ, ζ) plane with slope $-\delta$. This means that there are two options if we follow one of these curves: if $\delta \in \mathbb{Q}$ it closes itself or if $\delta \in \mathbb{R}\backslash\mathbb{Q}$ it densely fills the whole flux surface. Continuity of g_{h} over the torus implies that in order for $G(\varphi)$ to be non zero, either

$$A_k(L_\alpha, \varphi) = 0, \quad \text{if } \delta \in \mathbb{Q}, \tag{B.13}$$

or

$$\lim_{\alpha\to\infty} A_k(\alpha, \varphi) = 0, \quad \text{if } \delta \in \mathbb{R}\backslash\mathbb{Q}, \tag{B.14}$$

where L_α is the arc-length required for the curve of constant φ to close itself. However, with the exception of A_0 which is identically zero, A_k never annuls. This means that for $k \geq 1$, the constant of integration $G(\varphi)$ in (B.10) is 0. Hence, for $k \geq 1$, we can write the inverse of D_k as the operator

$$D_k^{-1} s = -\frac{\langle B^2 \rangle}{\hat{E}_\psi} \exp(A_k(\alpha, \varphi)) \times \int_0^\alpha s(\alpha', \varphi) \exp(-A_k(\alpha', \varphi)) \frac{\mathrm{d}\alpha'}{B^2(\alpha', \varphi)}, \tag{B.15}$$

and is straightforward to check that $D_k D_k^{-1} s = D_k^{-1} D_k s = s$. The operator D_0 is not invertible as it is identically zero for $\hat{E}_\psi = 0$ and $g_{\mathrm{h}} = G(\varphi)$ for $\hat{E}_\psi \neq 0$. Finally, we will study the invertibility of the operator Δ_k

$$\Delta_k = D_k - U_k \Delta_{k+1}^{-1} L_{k+1} \tag{B.16}$$

assuming that Δ_{k+1} is bounded and invertible. For this, first, we note that in the space of functions of interest (smooth periodic functions on the torus), using a Fourier basis $\{e^{\mathrm{i}(m\theta + nN_p\zeta)}\}_{m,n\in\mathbb{Z}}$, we can approximate any function $f(\theta, \zeta) = \sum_{m,n\in\mathbb{Z}} \hat{f}_{mn} e^{\mathrm{i}(m\theta+nN_p\zeta)}$ to arbitrary precision using an approximant $\tilde{f}(\theta, \zeta)$ with N_{m} modes, taking N_{m} sufficiently large. Hence, as they are bounded operators, we can approximate D_k, U_k, Δ_{k+1} and L_{k+1} (and therefore Δ_k) in (B.16) by square matrices of size N_{m}. Doing so, we can interpret the matrix representation of Δ_k as the Schur complement of the matrix

$$M_k = \begin{bmatrix} D_k & U_k \\ L_{k+1} & \Delta_{k+1} \end{bmatrix}. \tag{B.17}$$

It is well known from linear algebra that the Schur complement of M_k is invertible when both D_k and Δ_{k+1} are. Hence, for $k \geq 1$, the matrix representation of Δ_k can be inverted for any N_{m}, and thus Δ_k is also invertible. For $k = 0$, it is necessary to substitute one of the rows of $[D_k \;\; U_k]$ by the condition (36) so that M_k is invertible for any N_{m} and as Δ_1 can be inverted, also Δ_0 constructed in this way.

C. Fourier collocation method

We define our Fourier interpolant as

$$f^{(k)}(\theta, \zeta) = \boldsymbol{I}(\theta, \zeta) \cdot \boldsymbol{f}^{(k)} = \sum_{j'=0}^{N_\zeta - 1} \sum_{i'=0}^{N_\theta - 1} I_{i'j'}(\theta, \zeta) f^{(k)}(\theta_{i'}, \zeta_{j'}), \tag{C.1}$$

where $\boldsymbol{f}^{(k)} \in \mathbb{R}^{N_{\mathrm{fs}}}$ is the state vector containing $f^{(k)}(\theta_{i'}, \zeta_{j'})$. The entries of the vector $\boldsymbol{I}(\theta, \zeta)$ are the functions $I_{i'j'}(\theta, \zeta)$ given by,

$$I_{i'j'}(\theta, \zeta) = I^\theta_{i'}(\theta) I^\zeta_{j'}(\zeta), \tag{C.2}$$

$$I^\theta_{i'}(\theta) = \frac{1}{N_\theta} \sum_{m=-N_{\theta 1}/2}^{N_{\theta 2}/2 - 1} e^{\mathrm{i}m(\theta - \theta_{i'})}, \tag{C.3}$$

$$I^\zeta_{j'}(\zeta) = \frac{1}{N_\zeta} \sum_{n=-N_{\zeta 1}/2}^{N_{\zeta 2}/2 - 1} e^{N_p \mathrm{i}n(\zeta - \zeta_{j'})}, \tag{C.4}$$

and $N_{\theta 1} = N_\theta - N_\theta \mod 2$, $N_{\theta 2} = N_\theta + N_\theta \mod 2$, $N_{\zeta 1} = N_\zeta - N_\zeta \mod 2$, $N_{\zeta 2} = N_\zeta + N_\zeta$

mod 2 for some positive integers N_θ, N_ζ. Note that the interpolant is the only finite Fourier sum which interpolates the data, as $I^\theta_{i'}(\theta_i) = \delta_{ii'}$ and $I^\zeta_{j'}(\zeta_j) = \delta_{jj'}$. Inserting (C.1) in (32) and evaluating at grid points gives

$$\left(L_k f^{(k-1)} + D_k f^{(k)} + U_k f^{(k)}\right)\Big|_{(\theta_i,\zeta_j)} = \left(L_k \boldsymbol{I}\cdot\boldsymbol{f}^{(k-1)} + D_k \boldsymbol{I}\cdot\boldsymbol{f}^{(k)} + U_k \boldsymbol{I}\cdot\boldsymbol{f}^{(k+1)}\right)\Big|_{(\theta_i,\zeta_j)}. \tag{C.5}$$

Here, $L_k\boldsymbol{I}(\theta_i,\zeta_j)$, $D_k\boldsymbol{I}(\theta_i,\zeta_j)$ and $U_k\boldsymbol{I}(\theta_i,\zeta_j)$ are respectively the rows of $\boldsymbol{L}_k$, $\boldsymbol{D}_k$ and $\boldsymbol{U}_k$ associated to the grid point (θ_i,ζ_j). We can relate them to the actual positions they will occupy in the matrices choosing an ordenation of rows and columns. If we use the ordenation that relates respectively the row i_r and column i_c to the grid points (θ_i,ζ_j) and $(\theta_{i'},\zeta_{j'})$ as

$$i_\mathrm{r} = 1 + i + jN_\theta, \tag{C.6}$$
$$i_\mathrm{c} = 1 + i' + j'N_\theta, \tag{C.7}$$

for $i,i' = 0,1,\ldots,N_\theta - 1$ and $j,j' = 0,1,\ldots,N_\zeta - 1$. With this ordenation we define the elements of the row i_r and column i_c of the matrices $\boldsymbol{L}_k$, $\boldsymbol{D}_k$ and $\boldsymbol{U}_k$ to be

$$(\boldsymbol{L}_k)_{i_\mathrm{r}i_\mathrm{c}} = L_k I_{i'j'}(\theta_i,\zeta_j), \tag{C.8}$$
$$(\boldsymbol{D}_k)_{i_\mathrm{r}i_\mathrm{c}} = D_k I_{i'j'}(\theta_i,\zeta_j), \tag{C.9}$$
$$(\boldsymbol{U}_k)_{i_\mathrm{r}i_\mathrm{c}} = U_k I_{i'j'}(\theta_i,\zeta_j). \tag{C.10}$$

Explicitly,

$$L_k I_{i'j'}\Big|_{(\theta_i,\zeta_j)} = \frac{k}{2k-1}\left(\boldsymbol{b}\cdot\nabla I_{i'j'}\Big|_{(\theta_i,\zeta_j)} + \frac{k-1}{2}\,\boldsymbol{b}\cdot\nabla\ln B\Big|_{(\theta_i,\zeta_j)}\delta_{ii'}\delta_{jj'}\right), \tag{C.11}$$

$$D_k I_{i'j'}\Big|_{(\theta_i,\zeta_j)} = \frac{\hat{E}_\psi}{\langle B^2\rangle}\,\boldsymbol{B}\times\nabla\psi\cdot\nabla I_{i'j'}\Big|_{(\theta_i,\zeta_j)} + \frac{k(k+1)}{2}\hat{\nu}\delta_{ii'}\delta_{jj'}, \tag{C.12}$$

$$U_k I_{i'j'}\Big|_{(\theta_i,\zeta_j)} = \frac{k+1}{2k+3}\left(\boldsymbol{b}\cdot\nabla I_{i'j'}\Big|_{(\theta_i,\zeta_j)} + \frac{k+2}{2}\,\boldsymbol{b}\cdot\nabla\ln B\Big|_{(\theta_i,\zeta_j)}\delta_{ii'}\delta_{jj'}\right), \tag{C.13}$$

and

$$\boldsymbol{b}\cdot\nabla I_{i'j'}\Big|_{(\theta_i,\zeta_j)} = \frac{B(\theta_i,\zeta_j)}{B_\zeta + \iota B_\theta}\left(\iota\delta_{jj'}\,\frac{\mathrm{d}I^\theta_{i'}}{\mathrm{d}\theta}\Big|_{\theta_i} - \delta_{ii'}\,\frac{\mathrm{d}I^\zeta_{j'}}{\mathrm{d}\zeta}\Big|_{\zeta_j}\right) \tag{C.14}$$

$$\boldsymbol{B}\times\nabla\psi\cdot\nabla I_{i'j'}\Big|_{(\theta_i,\zeta_j)} = \frac{B^2(\theta_i,\zeta_j)}{B_\zeta + \iota B_\theta}\left(B_\zeta\delta_{jj'}\,\frac{\mathrm{d}I^\theta_{i'}}{\mathrm{d}\theta}\Big|_{\theta_i} - B_\theta\delta_{ii'}\,\frac{\mathrm{d}I^\zeta_{j'}}{\mathrm{d}\zeta}\Big|_{\zeta_j}\right) \tag{C.15}$$

Thus, we discretize (32) as

$$\boldsymbol{L}_k\boldsymbol{f}^{(k-1)} + \boldsymbol{D}_k\boldsymbol{f}^{(k)} + \boldsymbol{U}_k\boldsymbol{f}^{(k+1)} = \boldsymbol{s}^{(k)}, \tag{C.16}$$

for $k = 0,1\ldots,N_\xi$. We remark that, for $k=0$, the rows of $\boldsymbol{D}_0$ and $\boldsymbol{U}_0$ associated to the grid point $(\theta_i,\zeta_j) = (0,0)$, must be replaced by equation (36). Each state vector $\boldsymbol{f}^{(k)}$ for the Fourier interpolants contains the images $f^{(k)}(\theta_{i'},\zeta_{j'})$ at the grid points, ordered according to (C.7). Thus, we can solve (C.16) for $\boldsymbol{f}^{(k)}$ applying forward elimination (37) and then backward substitution (41). Finally, we remark that as all $\boldsymbol{f}^{(k)}$ are real, we only need the real part of (C.16).

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